Sensitivity analysis for shape perturbation of cavity or internal crack using BIE and adjoint variable approach

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Abstract

This paper deals with the application of the adjoint variable approach to sensitivity analysis of objective functions used for defect detection from knowledge of supplementary boundary data, in connexion with the use of BIE/BEM formulations for the relevant forward problem. The main objective is to establish expressions for crack shape sensitivity, based on the adjoint variable approach, that are suitable for BEM implementation.

In order to do so, it is useful to consider first the case of a cavity defect, for which such boundary-only sensitivity expressions are obtained for general initial geometry and shape perturbations. The analysis made in the cavity defect case is then seen to break down in the limiting case of a crack. However, a closer analysis reveals that sensitivity formulas suitable for BEM implementation can still be established. First, particular sensitivity formulas are obtained for special shape transformations (translation, rotation or expansion of the crack) for either two- or three-dimensional geometries which, except for the case of crack expansion together with dynamical governing equations, are made only of surface integrals (three-dimensional geometries) or line integrals (two-dimensional geometries). Next, arbitrary shape transformations are accommodated by using an additive decomposition of the transformation velocity over a tubular neighbourhood of the crack front, which leads to sensitivity formulas . This leads to sensitivity formulas involving integrals on the crack, the tubular neighbourhood and its boundary. Finally, the limiting case of the latter results when the tubular neighbourhood shrinks around the crack front is shown to yield a sensitivity formula involving the stress intensity factors of both the forward and the adjoint solutions. Classical path-independent integrals are recovered as special cases.

The main exposition is done in connexion with the scalar transient wave equation. The results are then extended to the linear time-domain elastodynamics framework. Linear static governing equations are contained as obvious special cases. Numerical results for crack shape sensitivity computation are presented for two-dimensional time-domain elastodynamics.

Key words: geometrical inverse problem, wave propagation, elastodynamics, adjoint variable approach, material derivative, defect identification, boundary integral equations, boundary element method.

1 Introduction

The consideration of sensitivity analysis of integral functionals with respect to shape parameters arises in many situations where a geometrical domain plays a primary role; shape optimization and inverse problems are the most obvious, as well as possibly the most important, of such instances.

It is well known that, apart from resorting to approximative techniques such as finite differences, shape sensitivity evaluation can be dealt with using either the direct differentiation approach or the adjoint variable approach (see e.g. Burczyński, 1993b), the present paper being focused on the latter. Besides, consideration of shape changes in otherwise (i.e. for fixed shape) linear problems makes it very attractive to use boundary integral equation (BIE) formulations, which constitute the minimal modelling as far as the geometrical support of unknown field variables is concerned.

In the BIE context, the direct differentiation approach rests primarily upon the material differentiation of the governing integral equations. This step has been studied by many researchers, from BIE formulation in either singular form (Barone and Yang, 1989; Mellings and Aliabadi, 1995) or regularized form (Bonnet, 1995b; Matsumoto, Tanaka, Miyagawa, and Ishii, 1993; Nishimura, Furukawa, and Kobayashi, 1992; Nishimura, 1995). Following this approach, the process of sensitivity computation needs the solution of as many new boundary-value problems as the numbers of shape parameters present. The fact that they all involve the same, original, governing operator reduces the computational effort to the building of new right-hand sides and the solution of linear systems by backsubstitution. The usual material differentiation formula for surface integrals is shown in Bonnet (1997) to be still valid when applied to strongly singular or hypersingular formulations. Thus, the direct differentiation approach is in particular applicable in the presence of cracks.

The adjoint variable approach is even more attractive, since it requires the solution of only one new boundary-value problem (the so-called adjoint problem) per integral functional present (often only one), whatever the number of shape parameters. In connexion with BIE formulations alone, the adjoint variable approach has been successfully applied to many shape sensitivity problems (see e.g. Aithal and Saigal, 1995; Bonnet, 1995a; Burczyński, 1993a; Burczyński and Fedelinski, 1992; Burczyński, Kane, and Balakrishna, 1995; Choi and Kwak, 1988; Meric, 1995). This relies heavily upon the possibility of formulating the final, analytical expression of the shape sensitivity of a given integral functional as a boundary integral that involves the values taken by the primary and adjoint states on the boundary. However, obtaining this boundary-only expression raises mathematical difficulties when the geometrical domain under consideration contains cracks or other geometrical singularities; non-integrable terms associated with e.g. crack tip singularity of field variables appear in some expressions.

This paper deals with the formulation of the adjoint variable method applied to sensitivity analysis, in connexion with the use of BIE formulations for the transient wave equation. Typical problems where this approach is useful are inverse problems of cavity or crack detection from transient wave measurements on a part of the external boundary, where the integral functionals considered express the gap between measured and computed data on the external boundary, e.g. in the form of a least-squares distance. However, the sensitivity results are derived for more general boundary integral functionals. The formulation of the adjoint problem and the corresponding boundary-only formula for the shape sensitivity of the functional are established for the case of an unknown cavity. The latter is then shown to become inconsistent in the limit when the cavity becomes a crack, due to the non-integrability of a certain domain integral, causing an integration-by-parts process to break down. However, resting on the analysis made for the case of a cavity, functional shape sensitivity expressions consistent with the use of BIE formulations and applicable to crack identification problems are derived in three different forms. Firstly, simple shape transformations (translations, rotations, expansion) are considered. Secondly, a sensitivity formula involving integrals on the crack, on an arbitrary tubular neighbourhood of the crack front and on its boundary is derived. Thirdly, the limiting case of the latter result when the tubular neighbourhood shrinks around the crack front is shown to yield a sensitivity formula involving the stress intensity factors of both the forward and the adjoint solutions. All sensitivity results presented here are obtained from the formulation of the continuous problem, i.e. are not directly obtained from the BIE formulations but are tailored for use in conjunction with the BEM. It is also possible to define adjoint problems and sensitivity results directly from the BIE formulations (Bonnet, 2001).

2 Motivation for shape sensitivity analysis

Consider a bounded domain B with external boundary S which contains a defect in the form of either a cavity V of boundary Γ (Fig.1a) or a crack with crack surface Γ (Fig.1b); Γ is not assumed to be simply connected (i.e. multiple defects are not ruled out). Let Ω denote the actual body (i.e.containing the defect): $\Omega = B \setminus V$ or $\Omega = B \setminus \Gamma$.

The framework adopted in this paper is that of transient linear wave propagation. Both scalar and vector (elastodynamic) cases are considered. In the interest of clarity, the investigation is first carried out in detail for scalar wave problems (sections 3 to 7). The corresponding developments and results for elastodynamics are then presented in section 8. Three-dimensional configurations are assumed unless explicitly stated otherwise.

The shape and position of the boundary Γ characterizing the defect are unknown. Assuming that

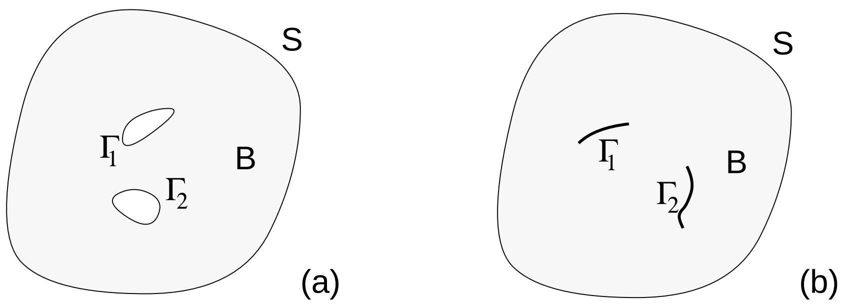

Figure 1: A body with internal defects: (a) cavities, (b) cracks

the defect surface is flux-free, the primary physical variable of interest u (e.g. acoustic pressure), termed 'potential', and its normal derivative $p = \partial u/\partial n$ are related by the field equation:

$$\Delta u - \frac{1}{c^2}\ddot{u} = 0 \qquad (\text{in } \Omega) \tag{1}$$

(where c is the wave velocity), the boundary conditions:

$$u = \bar{u} \quad (\text{on } S_u) \qquad p = \bar{p} \quad (\text{on } S_p) \qquad p = 0 \quad (\text{on } \Gamma) \tag{2}$$

(where S_u, S_p define a partition of S), and the initial conditions:

$$u = \dot{u} = 0 \qquad \text{in } \Omega, \text{ at } t = 0 \tag{3}$$

In the case of a crack, the variable u is allowed to jump across Γ; $[\![u]\!] \equiv u^+ - u^- \neq 0$. The problem thus defined is usually referred to as the *forward*, or *primary*, problem.

Consider the problem of determining the shape and position of the defect using experimental data and physical quantity governed by problem (1,2,3), as in ultrasonic measurements. The lack of information about V and Γ is compensated by some knowledge about u on S (redundant boundary data). Assume for example that a measurement $\hat{u}(\boldsymbol{x}, t)$ of u (resp. $\hat{p}(\boldsymbol{x}, t)$ of p) is available for $\boldsymbol{x} \in S_p$ (resp. $\boldsymbol{x} \in S_u$) and $t \in [0, T]$. The usual approach for finding Γ is the minimization of some distance J between the computed and measured quantities, e.g.

$$\mathcal{J}(\Gamma) = J(u_\Gamma, p_\Gamma, \Gamma) = \frac{1}{2}\int_0^T\!\!\int_{S_p} (\hat{u} - u_\Gamma)^2 \,\mathrm{d}S\,\mathrm{d}t + \frac{1}{2}\int_0^T\!\!\int_{S_u} (\hat{p} - p_\Gamma)^2 \,\mathrm{d}S\,\mathrm{d}t \tag{4}$$

where (u_Γ, p_Γ) pertains to the solution of problem (1,2,3) for a given Γ. Using classical optimization techniques, the minimization of $\mathcal{J}$ with respect to Γ needs in turn, for efficiency, the evaluation of the functional $\mathcal{J}$ and its gradient with respect to perturbations of Γ.

Other kinds of sensitivity problems with different motivations (e.g. optimization) can be considered as well. Let us thus introduce the following generic objective function:

$$\mathcal{J}(\Gamma) = J(u_\Gamma, p_\Gamma, \Gamma) = \int_0^T\!\!\int_{S_p} \varphi_u(u_\Gamma, \boldsymbol{x}, t) \,\mathrm{d}S\,\mathrm{d}t + \int_0^T\!\!\int_{S_u} \varphi_p(p_\Gamma, \boldsymbol{x}, t) \,\mathrm{d}S\,\mathrm{d}t \tag{5}$$

Since (i) functionals J of the type (5) depend only on boundary quantities, (ii) the forward problem (1,2,3) is linear and does not involve sources distributed over the domain Ω, and (iii) variations of boundary shapes are of primary concern, the boundary element method (recent expositions of which are e.g. Aliabadi, 2001; Bonnet, 1999; Wrobel, 2001) is adopted as the solution tool for the forward problem (1,2,3), and the adjoint problem as well later on.

3 Forward problem in terms of boundary integral equations

It is possible to distinguish two basic approaches for solving the forward problems formulated in the previous section by the boundary element method. One is based on the time-dependent fundamental solution (time-domain formulation), the other uses the time-independent fundamental solution together with the dual reciprocity technique. Both are abundantly documented, see e.g. the review papers by Beskos (1987, 1997) and the numerous references therein.

The first approach applied to the cavity problem leads to the following boundary integral equation in the time domain:

$$\frac{1}{2}u(\boldsymbol{x},t) + \int\!\!\!\!\!\!-_{\partial\Omega} H(\boldsymbol{x},\boldsymbol{y},t) \star u(\boldsymbol{y},t)\,\mathrm{d}S_y - \int_{\partial\Omega} G(\boldsymbol{x},\boldsymbol{y},t) \star p(\boldsymbol{y},t)\,\mathrm{d}S_y = 0 \tag{6}$$

where $G(\boldsymbol{x},\boldsymbol{y},t)$ is a time-dependent fundamental solution of wave equation, i.e. solves:

$$\Delta G - \frac{1}{c^2}\ddot{G} + \delta(\boldsymbol{y}-\boldsymbol{x})\delta(t) = 0, \qquad \boldsymbol{x},\boldsymbol{y} \in \mathbb{R}^m,\ m = 2 \text{ or } 3$$

and $H(\boldsymbol{x},\boldsymbol{y},t) = \boldsymbol{n}.\boldsymbol{\nabla}_y G(\boldsymbol{x},\boldsymbol{y},t)$ (the symbol $\star$ denotes time convolution). Numerical solution of the forward wave propagation problem is obtained after discretizing both space and time variations. The boundary is divided into boundary elements. The observation time is divided into time steps. The potential $u(\boldsymbol{y},t)$ and the flux $p(\boldsymbol{y},t)$ are approximated within each boundary element and each time step by suitable interpolation functions. After such discretization the boundary integral equation is transformed into an algebraic matrix equation which is solved step-by-step.

Alternatively, if the dual reciprocity approach (Partridge, Brebbia, and Wrobel, 1992) is used, the acceleration inside Ω is approximated by a set of A given co-ordinate functions $r^\alpha(\boldsymbol{y})$:

$$\ddot{u}(\boldsymbol{y},t) = \sum_{\alpha=1}^{A} \ddot{s}^\alpha(t) r^\alpha(\boldsymbol{y})$$

where $s^\alpha(t)$ is a set of unknown, time-dependent, functions. The boundary integral equation takes the form:

$$\begin{aligned}\frac{1}{2}u(\boldsymbol{x},t) &+ \int\!\!\!\!\!\!-_{\partial\Omega} H(\boldsymbol{x},\boldsymbol{y})u(\boldsymbol{y},t)\,\mathrm{d}S_y - \int_{\partial\Omega} G(\boldsymbol{x},\boldsymbol{y})p(\boldsymbol{y},t)\,\mathrm{d}S_y \\ &= \frac{1}{c^2}\sum_{\alpha=1}^{A}\Big\{\frac{1}{2}\tilde{u}^\alpha(\boldsymbol{x},t) + \int\!\!\!\!\!\!-_{\partial\Omega} H(\boldsymbol{x},\boldsymbol{y})\tilde{u}^\alpha(\boldsymbol{y},t)\,\mathrm{d}S_y - \int_{\partial\Omega} G(\boldsymbol{x},\boldsymbol{y})\tilde{p}^\alpha(\boldsymbol{y},t)\,\mathrm{d}S_y\Big\}\ddot{s}^\alpha(t)\end{aligned} \tag{7}$$

where $G(\boldsymbol{x},\boldsymbol{y})$ is the time-independent fundamental solution of the Laplace equation:

$$\Delta G + \delta(\boldsymbol{y}-\boldsymbol{x}) = 0, \qquad \boldsymbol{x},\boldsymbol{y} \in \mathbb{R}^m,\ m = 2 \text{ or } 3$$

and $\tilde{u}^\alpha(\boldsymbol{y},t)$ is a particular, known, solution to the field equation $\Delta\tilde{u}^\alpha = r^\alpha(\boldsymbol{y})$ and $\tilde{p}^\alpha(\boldsymbol{y},t)$ is the corresponding flux at the boundary.

Either equations (6) or (7) can be applied to the cavity problem. If these equations are used to the crack problem with collocation points $\boldsymbol{x}$ on both crack faces $\Gamma^\pm$, then two identical equations would be formed, with the resulting set of equations being singular. In order to overcome this problem without the use of the subdivision technique, which is not convenient in geometrical inverse problems and variable domains, a new independent equation for the flux, obtained by evaluating the normal derivative of the potential equation at collocation points $\boldsymbol{x} \in \Gamma$, is used. This flux BIE reads

$$\begin{aligned} p^\pm(\boldsymbol{x},t) &+ n_i^\pm(\boldsymbol{x}) \,=\!\!\!\!\!\!\int_\Gamma H_{,i}(\boldsymbol{x},\boldsymbol{y},t) \star [\![u]\!](\boldsymbol{y},t)\,\mathrm{d}S_y \\ &+ n_i^\pm(\boldsymbol{x}) \int_S \big[H_{,i}(\boldsymbol{x},\boldsymbol{y},t) \star u(\boldsymbol{y},t) - G_{,i}(\boldsymbol{x},\boldsymbol{y},t) \star p(\boldsymbol{y},t)\big]\,\mathrm{d}S_y = 0 \qquad (\boldsymbol{x} \in \Gamma^\pm) \end{aligned} \tag{8}$$

when obtained from the time-domain potential BIE (6), and

$$\begin{aligned} &p^\pm(\boldsymbol{x},t) + n_i^\pm(\boldsymbol{x}) \,=\!\!\!\!\!\!\int_\Gamma H_{,i}(\boldsymbol{x},\boldsymbol{y})[\![u]\!](\boldsymbol{y},t)\,\mathrm{d}S_y + n_i^\pm(\boldsymbol{x}) \int_S \big[H_{,i}(\boldsymbol{x},\boldsymbol{y})u(\boldsymbol{y},t) - G_{,i}(\boldsymbol{x},\boldsymbol{y})p(\boldsymbol{y},t)\big]\,\mathrm{d}S_y \\ &= \frac{1}{c^2}\sum_{\alpha=1}^{A}\Big\{\tilde{p}^\alpha(\boldsymbol{x},t) + n_i(\boldsymbol{x})\int_S \big[H_{,i}(\boldsymbol{x},\boldsymbol{y})\tilde{u}^\alpha(\boldsymbol{y},t) - G_{,i}(\boldsymbol{x},\boldsymbol{y})\tilde{p}^\alpha(\boldsymbol{y},t)\big]\,\mathrm{d}S_y\Big\}\ddot{s}^\alpha(t) \qquad (\boldsymbol{x} \in \Gamma^\pm) \end{aligned} \tag{9}$$

when obtained from the dual-reciprocity potential BIE (7), having used that that the particular solutions $\tilde{u}^\alpha$ is continuous across the crack. Hence, the forward problem for the embedded crack is formulated as either (6) collocated on S and (8) collocated on Γ (using a time-domain BIE formulation) or (7) collocated on S and (9) collocated on Γ (using a dual-reciprocity BIE formulation).

Note that the primary crack unknown in both flux equations is the jump $[\![u]\!](\boldsymbol{y},t)$; this is sufficient for the present purposes. However one might also use the so-called dual formulation (Portela, Aliabadi, and Rooke, 1992), whereby both the potential and the flux integral equations are considered for collocation points on Γ; in that case, u^+ and u^- are recovered separately. The dual formulation can be considered for the BIEs in either time-domain or dual-reciprocity forms.

Irrespective of the specific BIE formulation being used, S and Γ are divided into boundary elements, and potentials and fluxes within each element are approximated using the same spatial interpolation functions. In the time-domain formulation, a time interpolation is introduced as well, which results in a system of linear equations having a discrete convolution structure. Alternatively, in the dual-reciprocity formulation, the coefficients $\ddot{s}^\alpha(t)$ are expressed in terms of the unknown nodal accelerations. As a result, a system of ordinary differential equations in time is obtained. In all cases, a time-stepping scheme is finally performed.

4 Sensitivity analysis

Consider in the m-dimensional Euclidean space $\mathbb{R}^m$, $m = 2$ or 3, a body Ω_b whose shape depends on a finite number of shape parameters $\boldsymbol{b} = (b_1, b_2, \dots)$. Shape parameters are treated as time-like parameters using a continuum kinematics-type Lagrangian description and initial configuration Ω_0 conventionally associated with $\boldsymbol{b} = \boldsymbol{0}$ (Bonnet, 1995b; Burczyński, Kane, and Balakrishna, 1995; Petryk and Mróz, 1986):

$$\boldsymbol{x} \in \Omega_0 \rightarrow \boldsymbol{x}^b = \boldsymbol{\Phi}(\boldsymbol{x}, \boldsymbol{b}) \in \Omega_b \qquad \text{where} \quad (\forall \boldsymbol{x} \in \Omega_0),\ \boldsymbol{\Phi}(\boldsymbol{x}, \boldsymbol{0}) = \boldsymbol{x}$$

The geometrical transformation $\boldsymbol{\Phi}(\cdot, \boldsymbol{b})$ must possess a strictly positive Jacobian for any given $\boldsymbol{b}$. Since only first-order derivatives with respect to $\boldsymbol{b}$ are considered in this paper, attention is, without loss of generality, restricted to the consideration of a single shape parameter b.

The *initial transformation velocity* field $\boldsymbol{\theta}(\boldsymbol{x})$, defined by

$$\boldsymbol{\theta}(\boldsymbol{x}) = \frac{\partial \boldsymbol{\Phi}(\boldsymbol{x}, b)}{\partial \boldsymbol{b}}\Big|_{b=0}$$

is the 'initial' velocity of the 'material' point which coincides with the geometrical point $\boldsymbol{x}$ at 'time' $b = 0$.

The following relations hold between the total (or 'lagrangian', or 'material') derivative $\overset{\diamond}{f} = df/db$ and the partial (or 'eulerian') derivative $f' = \partial f / \partial b$ of any sufficiently regular function $f(\boldsymbol{x}, b)$:

$$\overset{\diamond}{f} = f' + \boldsymbol{\nabla} f.\boldsymbol{\theta} \qquad (\boldsymbol{\nabla} f)^{\diamond} = \boldsymbol{\nabla}(\overset{\diamond}{f}) - \boldsymbol{\nabla} f.\boldsymbol{\nabla}.\boldsymbol{\theta} \tag{10}$$

The material derivatives of generic domain and boundary integrals are expressed by (see e.g. Petryk and Mróz, 1986):

$$\frac{d}{db}\int_{\Omega} f \,\mathrm{d}\Omega = \int_{\Omega} (\overset{\diamond}{f} + f \operatorname{div} \boldsymbol{\theta}) \,\mathrm{d}\Omega \qquad \Omega\text{: any domain} \tag{11}$$

$$\frac{d}{db}\int_{S} f \,\mathrm{d}S = \int_{S} (\overset{\diamond}{f} + f \operatorname{div}_S \boldsymbol{\theta}) \,\mathrm{d}S \qquad S\text{: any surface} \tag{12}$$

The surface divergence is defined by $\operatorname{div}_S \boldsymbol{\theta} = \operatorname{div} \boldsymbol{\theta} - \boldsymbol{n}.\boldsymbol{\nabla}\boldsymbol{\theta}.\boldsymbol{n}$, where $\boldsymbol{n}$ is the unit normal vector.

One assumes here that the external boundary S and its neighbourhood is unaffected by the shape transformation, so $\boldsymbol{\theta} = \boldsymbol{0}$ and $\boldsymbol{\nabla}\boldsymbol{\theta} = \boldsymbol{0}$ on S. However, this is not true when emerging cracks are considered: in this case, $\boldsymbol{\theta}$ and $\boldsymbol{\nabla}\boldsymbol{\theta}$ do not vanish on some neighbourhood of the emerging point (or edge in 3-D problems).

5 Shape sensitivity: adjoint problem and domain integral formulation

Introduce the following Lagrangian:

$$
\begin{aligned}
\mathcal{L}(u,v,p,q,\Gamma) = J(u,p,\Gamma) &+ \int_0^T\!\!\int_\Omega \Big\{ \boldsymbol{\nabla} u.\boldsymbol{\nabla} v + \frac{1}{c^2}\ddot{u}v \Big\}\,\mathrm{d}\Omega\,\mathrm{d}t \\
&- \int_0^T\!\!\int_{S_u} (u-\bar{u})q\,\mathrm{d}S\,\mathrm{d}t - \int_0^T\!\!\int_{S_u} pv\,\mathrm{d}S\,\mathrm{d}t - \int_0^T\!\!\int_{S_p} \bar{p}v\,\mathrm{d}S\,\mathrm{d}t
\end{aligned} \tag{13}
$$

in which the weak formulation of the forward wave problem (1,2,3) appears as an equality constraint term added to the objective function J, the Lagrange multipliers being the trial potential v and flux q.

Taking into account Eqs. (10)–(12), the total material derivative of the Lagrangian (13) with respect to a variation of the domain can be expressed as:

$$
\begin{aligned}
\frac{d}{db}\mathcal{L}(u,v,p,q,\Gamma) = &\int_0^T\!\!\int_\Omega \Big\{ \boldsymbol{\nabla} \overset{\diamond}{u} .\boldsymbol{\nabla} v + \frac{1}{c^2} \overset{\diamond}{\ddot{u}}\, v \Big\}\,\mathrm{d}\Omega\,\mathrm{d}t \\
&- \int_0^T\!\!\int_{S_u} q\, \overset{\diamond}{u}\;\mathrm{d}S\,\mathrm{d}t - \int_0^T\!\!\int_{S_u} \Big(v - \frac{\partial\varphi_p}{\partial p}\Big)\, \overset{\diamond}{p}\;\mathrm{d}S\,\mathrm{d}t + \int_0^T\!\!\int_{S_p} \frac{\partial\varphi_u}{\partial u}\, \overset{\diamond}{u}\;\mathrm{d}S\,\mathrm{d}t \\
&+ \int_0^T\!\!\int_\Omega \Big\{ \Big[\boldsymbol{\nabla} u.\boldsymbol{\nabla} v + \frac{1}{c^2}\ddot{u}v \Big] \operatorname{div}\boldsymbol{\theta} - (\boldsymbol{\nabla} u \otimes \boldsymbol{\nabla} v + \boldsymbol{\nabla} v \otimes \boldsymbol{\nabla} u) : \boldsymbol{\nabla}\boldsymbol{\theta} \Big\}\,\mathrm{d}\Omega\,\mathrm{d}t
\end{aligned} \tag{14}
$$

Note that the terms containing $(\overset{\diamond}{v}, \overset{\diamond}{v})$ do not appear in this result: they merely reproduce the forward problem constraint on (u,p) and thus collectively vanish if (u,p) is the solution to (1,2,3).

For cracks, the partial derivative $(\boldsymbol{\nabla} u)'$ has generally a $r^{-3/2}$ singularity along the crack edge $\mathrm{d}\Gamma$, while $\boldsymbol{\nabla}(\overset{\diamond}{u})$ and $\boldsymbol{\nabla} u$ have the same $r^{-1/2}$ singularity, where r is the distance to $\mathrm{d}\Gamma$. For this reason, the total derivative $\overset{\diamond}{u}$ has been introduced in (14) instead of the partial derivative u'. The derivations made in this section are therefore valid for both cavity and crack problems.

At this point, it is useful to remark that since the initial conditions $u(\cdot,0) = \dot{u}(\cdot,0)$ hold for any location of the assumed defect, one should assume $\overset{\diamond}{u}(\cdot,0) = \overset{\diamond}{\dot{u}}(\cdot,0)$ as well. One then has:

$$
\int_0^T \ddot{u}v\,\mathrm{d}t = (\dot{u}v - \dot{v}u)\big|_{t=T} + \int_0^T u\ddot{v}\,\mathrm{d}t \tag{15}
$$

$$
\int_0^T \overset{\diamond}{\ddot{u}}\, v\,\mathrm{d}t = (\overset{\diamond}{\dot{u}}\, v - \dot{v}\, \overset{\diamond}{u})\big|_{t=T} + \int_0^T \overset{\diamond}{u}\, \ddot{v}\,\mathrm{d}t \tag{16}
$$

In equation (14), the trial function v is now chosen so that the terms which contain $\overset{\diamond}{u}$ combine to zero for any $\overset{\diamond}{u}$. Using Eq. (15), one gets:

$$
\begin{aligned}
&\int_0^T\!\!\int_\Omega \Big\{ \boldsymbol{\nabla} v.\boldsymbol{\nabla} \overset{\diamond}{u} + \frac{1}{c^2}\ddot{v}\, \overset{\diamond}{u} \Big\}\,\mathrm{d}\Omega\,\mathrm{d}t + \int_\Omega (\overset{\diamond}{\dot{u}}\, v - \dot{v}\, \overset{\diamond}{u})\big|_{t=T}\,\mathrm{d}\Omega \\
&\quad - \int_0^T\!\!\int_{S_u} q\, \overset{\diamond}{u}\;\mathrm{d}S\,\mathrm{d}t - \int_0^T\!\!\int_{S_u} \Big(v - \frac{\partial\varphi_p}{\partial p}\Big)\, \overset{\diamond}{p}\;\mathrm{d}S\,\mathrm{d}t + \int_0^T\!\!\int_{S_p} \frac{\partial\varphi_u}{\partial u}\, \overset{\diamond}{u}\;\mathrm{d}S\,\mathrm{d}t = 0 \qquad (\forall\, \overset{\diamond}{u}, \overset{\diamond}{p})
\end{aligned} \tag{17}
$$

This last result is interpreted as the weak formulation of the *adjoint problem*, whereby the unknowns v, q solve the wave equation (1) together with the boundary conditions

$$u = \frac{\partial \varphi_p}{\partial p} \quad (\text{on } S_p) \qquad q = -\frac{\partial \varphi_u}{\partial u} \quad (\text{on } S_u) \qquad q = 0 \quad (\text{on } \Gamma) \tag{18}$$

and the *final* conditions

$$v = \dot{v} = 0 \qquad (\text{in } \Omega, \text{ at } t = T) \tag{19}$$

The adjoint problem (1,18,19) appears to be, as is generally the case, a backward evolution problem. It can be solved in the same way as the forward problem (1,2,3), i.e. using either the time domain formulation (6) or the dual reciprocity formulation (7), but with time reversed.

Finally, noting that initial conditions (3), (19) imply:

$$\int_0^T \ddot{u}_\Gamma v_\Gamma \, \mathrm{d}t = \dot{u}_\Gamma v_\Gamma \big|_{t=0}^{t=T} - \int_0^T \dot{u}_\Gamma \dot{v}_\Gamma \, \mathrm{d}t = -\int_0^T \dot{u}_\Gamma \dot{v}_\Gamma \, \mathrm{d}t$$

equation (14) allows to express the derivative of J in terms of the primary and adjoint solutions:

$$\begin{aligned} \frac{d\mathcal{J}}{db}(\Gamma) &= \frac{d}{db}\mathcal{L}(u_\Gamma, v_\Gamma, p_\Gamma, q_\Gamma, \Gamma) \\ &= \int_0^T \int_\Omega \Big\{ \Big[\boldsymbol{\nabla} u_\Gamma . \boldsymbol{\nabla} v_\Gamma - \frac{1}{c^2} \dot{u}_\Gamma \dot{v}_\Gamma \Big] \operatorname{div} \boldsymbol{\theta} - (\boldsymbol{\nabla} u_\Gamma \otimes \boldsymbol{\nabla} v_\Gamma + \boldsymbol{\nabla} v_\Gamma \otimes \boldsymbol{\nabla} u_\Gamma) : \boldsymbol{\nabla} \boldsymbol{\theta} \Big\} \, \mathrm{d}\Omega \, \mathrm{d}t \end{aligned} \tag{20}$$

6 Shape sensitivity: boundary integral formulation (cavity problem)

The formula (20) for the sensitivity of $\mathcal{J}$ is expressed by a domain integral. It is therefore not suitable for BEM-based computations. This section aims to show that Eq. (20) applied to the cavity problem can be converted into an equivalent, boundary-only, expression.

This step requires integrations by parts. First, it is easy to prove (for example using component notation) that, for arbitrary (sufficiently smooth) scalar fields u, v:

$$\begin{aligned} &(\boldsymbol{\nabla} u \otimes \boldsymbol{\nabla} v + \boldsymbol{\nabla} v \otimes \boldsymbol{\nabla} u) : \boldsymbol{\nabla} \boldsymbol{\theta} \\ &\qquad = \operatorname{div} [(\boldsymbol{\nabla} u \otimes \boldsymbol{\nabla} v + \boldsymbol{\nabla} v \otimes \boldsymbol{\nabla} u) . \boldsymbol{\theta}] - [(\Delta u) \boldsymbol{\nabla} v + (\Delta v) \boldsymbol{\nabla} u + \boldsymbol{\nabla} (\boldsymbol{\nabla} u . \boldsymbol{\nabla} v)] . \boldsymbol{\theta} \end{aligned}$$

Hence, since (u, v) in fact satisfy the field equation (1) and the initial conditions (3), (19), one has:

$$\int_0^T [(\Delta u) \boldsymbol{\nabla} v + (\Delta v) \boldsymbol{\nabla} u] . \boldsymbol{\theta} \, \mathrm{d}t = -\frac{1}{c^2} \int_0^T [\dot{u} \boldsymbol{\nabla} \dot{v} + \dot{v} \boldsymbol{\nabla} \dot{u}] . \boldsymbol{\theta} \, \mathrm{d}t$$

and hence:

$$\begin{aligned} &\int_0^T \Big\{ \Big[\boldsymbol{\nabla} u . \boldsymbol{\nabla} v - \frac{1}{c^2} \dot{u} \dot{v} \Big] \operatorname{div} \boldsymbol{\theta} - (\boldsymbol{\nabla} u \otimes \boldsymbol{\nabla} v + \boldsymbol{\nabla} v \otimes \boldsymbol{\nabla} u) : \boldsymbol{\nabla} \boldsymbol{\theta} \Big\} \, \mathrm{d}t \\ &\qquad = \int_0^T \operatorname{div} \Big[\Big(\boldsymbol{\nabla} u . \boldsymbol{\nabla} v - \frac{1}{c^2} \dot{u} \dot{v} \Big) \boldsymbol{\theta} - (\boldsymbol{\nabla} u \otimes \boldsymbol{\nabla} v + \boldsymbol{\nabla} v \otimes \boldsymbol{\nabla} u) . \boldsymbol{\theta} \Big] \, \mathrm{d}t \end{aligned} \tag{21}$$

This identity is then substituted into Eq. (20). Under the condition that the integral of the right-hand side of (21) is convergent (this provision will prove important for crack problems), application of the divergence formula yields the following boundary-only expression for $\mathrm{d}\mathcal{J}/\mathrm{d}b$:

$$\frac{d\mathcal{J}}{db}(\Gamma) = \int_0^T \int_{\partial\Omega} \Big\{ \Big[\boldsymbol{\nabla} u_\Gamma . \boldsymbol{\nabla} v_\Gamma - \frac{1}{c^2} \dot{u}_\Gamma \dot{v}_\Gamma \Big] \theta_n - (q_\Gamma \boldsymbol{\nabla} u_\Gamma + p_\Gamma \boldsymbol{\nabla} v_\Gamma) . \boldsymbol{\theta} \Big\} \, \mathrm{d}S \, \mathrm{d}t \tag{22}$$

(having put $\theta_n = \boldsymbol{\theta}.\boldsymbol{n}$). An alternative form of the above expression can be obtained by splitting gradients into tangential gradient $\boldsymbol{\nabla}_S$ and normal derivative according to the definition $\boldsymbol{\nabla}_S w = \boldsymbol{\nabla} w - (\boldsymbol{\nabla} w.\boldsymbol{n})\boldsymbol{n}$. It reads:

$$\frac{d\mathcal{J}}{db}(\Gamma) = \int_0^T \int_{\partial\Omega} \Big\{ \Big[\boldsymbol{\nabla}_S u_\Gamma . \boldsymbol{\nabla}_S v_\Gamma - pq - \frac{1}{c^2} \dot{u}_\Gamma \dot{v}_\Gamma \Big] \theta_n - (q_\Gamma \boldsymbol{\nabla}_S u_\Gamma + p_\Gamma \boldsymbol{\nabla}_S v_\Gamma) . \boldsymbol{\theta} \Big\} \, \mathrm{d}S \, \mathrm{d}t \tag{23}$$

Equation (22) and its variant form (23) hold for any domain Ω. For cavity identification problems, one has $\Omega = B \setminus V$, $\boldsymbol{\theta} = \boldsymbol{0}$ on S (external boundary unperturbed) and $p = q = 0$ on the cavity boundary Γ, so that Eq. (22) reduces to:

$$\frac{d\mathcal{J}}{db}(\Gamma) = \int_0^T \int_{\Gamma} \Big[\boldsymbol{\nabla}_S u_\Gamma . \boldsymbol{\nabla}_S v_\Gamma - \frac{1}{c^2} \dot{u}_\Gamma \dot{v}_\Gamma \Big] \theta_n \, \mathrm{d}S \, \mathrm{d}t \tag{24}$$

Formula (24) allows the computation of the derivatives of any objective functional $\mathcal{J}$ of the type (5) with respect to shape parameters. In particular, since $\boldsymbol{\nabla}_S u_\Gamma$, $\boldsymbol{\nabla}_S v_\Gamma$ are known from the knowledge of u_Γ and v_Γ on Γ only, the sensitivity (24) is computable directly from the BEM solution of the primary and adjoint problems.

7 Shape sensitivity: boundary integral formulation (crack problem)

Consider now the case where the unknown defect is a crack, i.e. the limiting case of a cavity bounded by two surfaces Γ^+ and Γ^- identical and of opposite orientations (Fig. 2). It is tempting to still apply Eq. (24) to compute sensitivities with respect to crack location perturbations. However, Eq. (24) is not applicable to cracks. For instance, consider a domain shape transformation such that $\theta_n = \boldsymbol{0}$ on the crack surface Γ. This means that crack perturbations along the tangent plane at the crack front (i.e. crack extensions) are allowed. But then Eq. (24) gives $\mathrm{d}\mathcal{J}/\mathrm{d}b = 0$, which is certainty not true in general. In contrast, when Γ is the piecewise smooth boundary of a cavity, $\theta_n = \boldsymbol{0}$ implies that the cavity is unperturbed.

This apparent paradox is due to the fact that, for cracks, u and v behave like $r^{1/2}$ in the vicinity of the crack front (r: distance to the nearest point on the crack front). Hence, the divergence in the right-hand side of (21) is integrable only away from the crack front, so that the divergence formula cannot be applied for the entire domain Ω.

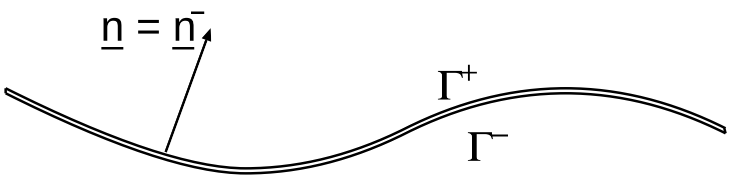

Figure 2: A crack bounded by two almost identical surfaces Γ^+ and Γ^-.

This section aims at showing how these difficulties can be overcome. For special cases of domain transformations, the domain integral disappears or is easily transformed (section 7.1), whereas the general case is handled by isolating a neighbourhood of the crack front and performing either an additive decomposition of the transformation velocity field (section 7.2) or a limiting process (section 7.3). Both approaches yields a fully general three-dimensional sensitivity formula; the former is in integral-invariant form and involves a residual domain integral while the latter uses the primary and adjoint singularity factors without any domain integration.

7.1 Special cases of domain transformations

Isolate a neighbourhood $D \subset \Omega$ of the crack bounded by the surface $\partial D = C$ (Fig. 3) and consider the transformation velocity fields $\boldsymbol{\theta}$ associated with special shape transformations of the crack: (a) translation of D, (b) expansion of D and (c) rotation of D. These shape transformations are continuously extended so that $\boldsymbol{\theta} = \mathbf{0}$, $\boldsymbol{\nabla\theta} = \mathbf{0}$ on S.

Then, Eq. (22) is valid for the subdomain $\Omega \setminus D$ while advantage is taken of the special form of $\boldsymbol{\theta}$ in D:

(a) Translation: $\boldsymbol{\theta} = \boldsymbol{\theta}_0$ (constant) in D, hence $\boldsymbol{\nabla\theta} = \mathbf{0}$, $\operatorname{div}\boldsymbol{\theta} = 0$ in D;

(b) Expansion with respect to the origin: $\boldsymbol{\theta} = \eta\boldsymbol{y}$ (η: expansion coefficient) so that $\boldsymbol{\nabla\theta} = \eta\boldsymbol{I}$, $\operatorname{div}\boldsymbol{\theta} = m\eta$ (m: space dimensionality) in D. In this case, the domain integral over D becomes:

$$\eta \int_D \Big\{(m-2)\boldsymbol{\nabla} u_\Gamma.\boldsymbol{\nabla} v_\Gamma - \frac{m}{c^2}\dot{u}_\Gamma\dot{v}_\Gamma\Big\}\,\mathrm{d}\Omega = \eta(m-2)\int_C p_\Gamma v_\Gamma\,\mathrm{d}S - \frac{2\eta}{c^2}\int_D \dot{u}_\Gamma\dot{v}_\Gamma\,\mathrm{d}\Omega$$

(c) Rotation: $\boldsymbol{\theta} = \boldsymbol{\Omega y}$ ($\boldsymbol{\Omega}$: constant tensor such that $\boldsymbol{\Omega} + \boldsymbol{\Omega}^T = \mathbf{0}$) so that $\boldsymbol{\nabla\theta} + \boldsymbol{\nabla\theta}^T = \mathbf{0}$ and $\operatorname{div}\boldsymbol{\theta} = 0$. Then, the domain integral in Eq. (20) vanishes.

Hence, using the exterior normal to SC, i.e. interior to $\Omega \setminus D$, cases (a), (b) and (c) are gathered

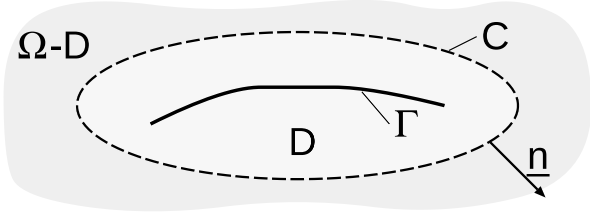

Figure 3: A crack Γ with a neighbourhood D

in the following result:

$$\frac{d\mathcal{J}}{db}(\Gamma) = \int_0^T \int_C \Big\{ \Big[\frac{1}{c^2} \dot{u}_\Gamma \dot{v}_\Gamma - \boldsymbol{\nabla} u_\Gamma . \boldsymbol{\nabla} v_\Gamma \Big] \theta_n + (\boldsymbol{\nabla} u_\Gamma . \boldsymbol{\theta}) q_\Gamma + (\boldsymbol{\nabla} v_\Gamma . \boldsymbol{\theta}) p_\Gamma \Big\} \, \mathrm{d}S \, \mathrm{d}t \\ + \eta(m-2) \int_C p_\Gamma v_\Gamma \, \mathrm{d}S - \frac{2\eta}{c^2} \int_D \ddot{u}_\Gamma v_\Gamma \, \mathrm{d}\Omega \quad (25)$$

where $\boldsymbol{\theta}$ is as defined in cases (a), (b), (c) above. The last two integrals in equation (25) appear only for the case (b).

The neighbourhood D of boundary S surrounding the crack is arbitrary. In case (b), due to the presence of the domain integral over D, the sensitivity of the functional J, as expressed by equation (25), is neither a true boundary-only expression, nor true path-independent integral, even if it does not depend on the choice of the surface C.

The special domain transformations considered here follow the idea introduced by Dems and Mróz (1986, 1995) for elastostatics and harmonic problems. They proved that when the transformation of the problem domain corresponds to translation, rotation or scale change then the class of conservation rules and associated path-independent integrals can be derived. This idea was numerically implemented using boundary elements for sensitivity analysis of cracks (Burczyński and Polch, 1994) and cavities (Burczyński and Habarta, 1995) in static problems. The considerations presented in this section are then an extension of previous works to time-domain dynamical problems.

7.2 Additive decomposition of transformation velocity near the crack front

To accommodate the general three-dimensional case with arbitrary crack shape perturbations, let the domain Ω be partitioned into $\Omega = \tilde{\Omega} \cup (D \setminus \Gamma)$, where D is a tubular neighbourhood of the crack front $\partial\Gamma$ bounded by the tubular surface Σ and $\tilde{\Omega} = \Omega \setminus \bar{D}$ (figure 4); in addition, let $\tilde{\Gamma} = \Gamma \setminus \bar{D}$.

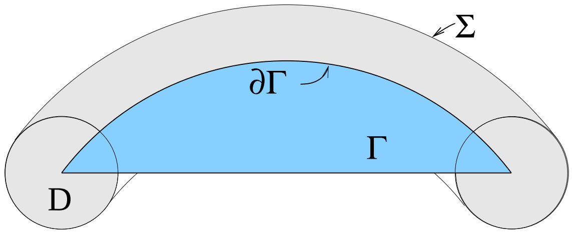

Figure 4: Crack Γ and tubular neighbourhood D of $\partial\Gamma$.

Introduction of this splitting into Eq. (20) yields:

$$\begin{aligned}\frac{d\mathcal{J}}{db}(\Gamma) &= \int_0^T\!\!\int_{\tilde{\Omega}} \Big\{ \Big[\boldsymbol{\nabla} u_\Gamma . \boldsymbol{\nabla} v_\Gamma - \frac{1}{c^2}\dot{u}_\Gamma \dot{v}_\Gamma \Big] \operatorname{div} \boldsymbol{\theta} - (\boldsymbol{\nabla} u_\Gamma \otimes \boldsymbol{\nabla} v_\Gamma + \boldsymbol{\nabla} v_\Gamma \otimes \boldsymbol{\nabla} u_\Gamma) : \boldsymbol{\nabla}\boldsymbol{\theta} \Big\} \,\mathrm{d}\Omega \,\mathrm{d}t \\ &+ \int_0^T\!\!\int_D \Big\{ \Big[\boldsymbol{\nabla} u_\Gamma . \boldsymbol{\nabla} v_\Gamma - \frac{1}{c^2}\dot{u}_\Gamma \dot{v}_\Gamma \Big] \operatorname{div} \boldsymbol{\mu} - (\boldsymbol{\nabla} u_\Gamma \otimes \boldsymbol{\nabla} v_\Gamma + \boldsymbol{\nabla} v_\Gamma \otimes \boldsymbol{\nabla} u_\Gamma) : \boldsymbol{\nabla}\boldsymbol{\mu} \Big\} \,\mathrm{d}\Omega \,\mathrm{d}t \\ &+ \int_0^T\!\!\int_D \Big\{ \Big[\boldsymbol{\nabla} u_\Gamma . \boldsymbol{\nabla} v_\Gamma - \frac{1}{c^2}\dot{u}_\Gamma \dot{v}_\Gamma \Big] \operatorname{div} \tilde{\boldsymbol{\theta}} - (\boldsymbol{\nabla} u_\Gamma \otimes \boldsymbol{\nabla} v_\Gamma + \boldsymbol{\nabla} v_\Gamma \otimes \boldsymbol{\nabla} u_\Gamma) : \boldsymbol{\nabla}\tilde{\boldsymbol{\theta}} \Big\} \,\mathrm{d}\Omega \,\mathrm{d}t \end{aligned} \tag{26}$$

having put

$$\boldsymbol{\mu} = \begin{cases} \boldsymbol{\theta} & \text{in } \tilde{\Omega} \\ \boldsymbol{\theta} - \tilde{\boldsymbol{\theta}} & \text{in } D_i \ (i = 1, 2) \end{cases} \tag{27}$$

where $\tilde{\boldsymbol{\theta}}$ denotes an arbitrarily chosen extension over D of the restriction $\boldsymbol{\theta}(s)$ of $\boldsymbol{\theta}$ on $\partial\Gamma$. By construction $\boldsymbol{\mu} = O(r)$, which makes the right-hand side of (21) integrable in that case. Hence, identity (21) followed with application of the divergence formula is used for the first two integrals in (26) above, resulting in:

$$\begin{aligned}\frac{d\mathcal{J}}{db}(\Gamma) &= \int_0^T\!\!\int_{\Gamma} \Big[\boldsymbol{\nabla}_S u_\Gamma . \boldsymbol{\nabla}_S v_\Gamma - \frac{1}{c^2}\dot{u}_\Gamma \dot{v}_\Gamma \Big] (\boldsymbol{\mu}.\boldsymbol{n}) \,\mathrm{d}S \,\mathrm{d}t \\ &+ \int_0^T\!\!\int_{\Sigma} \Big[\Big(\boldsymbol{\nabla} u_\Gamma . \boldsymbol{\nabla} v_\Gamma - \frac{1}{c^2}\dot{u}_\Gamma \dot{v}_\Gamma \Big) (\tilde{\boldsymbol{\theta}}.\boldsymbol{n}) - (p_\Gamma \boldsymbol{\nabla} v_\Gamma + q_\Gamma \boldsymbol{\nabla} u_\Gamma).\tilde{\boldsymbol{\theta}} \Big] \,\mathrm{d}S \,\mathrm{d}t \\ &+ \int_0^T\!\!\int_D \Big\{ \Big[\boldsymbol{\nabla} u_\Gamma . \boldsymbol{\nabla} v_\Gamma - \frac{1}{c^2}\dot{u}_\Gamma \dot{v}_\Gamma \Big] \operatorname{div} \tilde{\boldsymbol{\theta}} - (\boldsymbol{\nabla} u_\Gamma \otimes \boldsymbol{\nabla} v_\Gamma + \boldsymbol{\nabla} v_\Gamma \otimes \boldsymbol{\nabla} u_\Gamma) : \boldsymbol{\nabla}\tilde{\boldsymbol{\theta}} \Big\} \,\mathrm{d}\Omega \,\mathrm{d}t \end{aligned} \tag{28}$$

Note that the integral over Σ, for which the normal $\boldsymbol{n}$ exterior to D is chosen, is the net result of two contributions arising from domain integrations over $\tilde{\Omega}$ (velocity $\boldsymbol{\theta}$, normal $-\boldsymbol{n}$) and D (velocity $\boldsymbol{\mu}$, normal $\boldsymbol{n}$) respectively. Besides, the integral on Γ is convergent since $\boldsymbol{\mu}$ is built so as to vanish at the crack tips.

Equation (28) holds independently of the tubular neighbourhood D chosen, although it is not in general path-independent in the sense that a domain integral over D is involved as well and must be computed in practice.

For two-dimensional problems, Eq. (28) can be given a simpler form. The tubular neighbourhood D degenerates into disjoint neighbourhoods D_i $(i = 1, 2)$ of the two crack tips $\boldsymbol{x}^i$, bounded

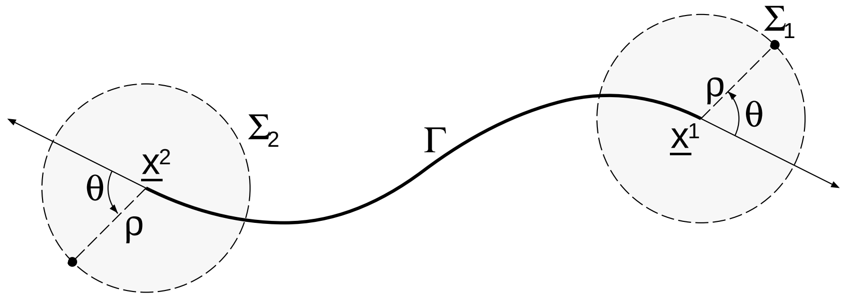

Figure 5: Two-dimensional case: geometrical notation; local polar coordinates (r, ϕ) associated with the crack tips $\boldsymbol{x}^{1,2}$.

by curves Σ_i (figure 5). One can then take $\tilde{\boldsymbol{\theta}} = \boldsymbol{\theta}^i$ on D_i, where the constant vector $\boldsymbol{\theta}^i$ denotes the value $\boldsymbol{\theta}(\boldsymbol{x}^i)$ of the transformation velocity at crack tip i. With this choice, $\boldsymbol{\nabla}\tilde{\boldsymbol{\theta}} = \boldsymbol{0}$ on D and the domain integral over D in Eq. (28) vanishes, yielding the sensitivity formula:

$$\frac{d\mathcal{J}}{db}(\Gamma) = \int_0^T \int_\Gamma \left[\!\!\left[\frac{du_\Gamma}{ds}\frac{dv_\Gamma}{ds} - \frac{1}{c^2}\dot{u}_\Gamma \dot{v}_\Gamma \right]\!\!\right] (\boldsymbol{\mu}.\boldsymbol{n}) \,\mathrm{d}s \,\mathrm{d}t$$
$$- \sum_{i=1}^{2} \int_0^T \int_{C_i} \left\{ \left[\frac{du_\Gamma}{ds}\frac{dv_\Gamma}{ds} - p_\Gamma q_\Gamma - \frac{1}{c^2}\dot{u}_\Gamma \dot{v}_\Gamma \right] (\boldsymbol{\theta}^i.\boldsymbol{n}) - (q_\Gamma \frac{du_\Gamma}{ds} + p_\Gamma \frac{dv_\Gamma}{ds})\boldsymbol{\theta}^i.\boldsymbol{\tau} \right\} \mathrm{d}s \,\mathrm{d}t \quad (29)$$

where $\boldsymbol{\mu}$ is still defined by (27), s denotes the arc length coordinate along Γ or Σ_i and $\boldsymbol{\tau}$ is the unit tangent vector on Σ_i oriented in the direction of increasing s.

The sensitivity expressions (28) and (29) are general in that they hold for any sufficiently smooth transformation velocity $\boldsymbol{\theta}$ and are not restricted to simple shape transformations.

For the special case of a crack extension, one has $\theta_n = 0$ on Γ and the integral over Γ thus reduces to

$$- \sum_{i=1}^{2} \int_0^T \int_{\Gamma_i} \left[\!\!\left[\boldsymbol{\nabla}_S u . \boldsymbol{\nabla}_S v - \frac{1}{c^2}\dot{u}\dot{v} \right]\!\!\right] (\boldsymbol{\theta}^i.\boldsymbol{n}) \,\mathrm{d}S \,\mathrm{d}t \quad (30)$$

(note that $\boldsymbol{\theta}^i.\boldsymbol{n} = 0$ vanishes at the tip $\boldsymbol{x}^i$, which makes the above integral convergent). If Γ_i are straight, then $\boldsymbol{\theta}^i.\boldsymbol{n} = 0$ on Γ_i and Eq. (29) looks like the usual J-integral; see section 10 for additional comments.

In three-dimensional situations, due to both the curvature of $\mathrm{d}\Gamma$ and the variability of $\boldsymbol{\theta}$ along $\mathrm{d}\Gamma$, any choice of $\tilde{\boldsymbol{\theta}}$ will have nonzero gradient and divergence in D, hence no simple choice of $\tilde{\boldsymbol{\theta}}$ is expected to make the domain integral in (28) vanish.

7.3 Sensitivity formulation in terms of singularity factors

Equation (28) holds irrespective of the tubular neighbourhood D chosen. In particular, in an effort to avoid the domain integration,one is led to to investigate the limiting form of Eq. (28) as D

vanishes. To do so, let $D_\varepsilon = \{\boldsymbol{x}, \text{dist}(\boldsymbol{x}, \partial\Gamma) \le \varepsilon\}$ denote the tubular neighbourhood of $\partial\Gamma$ having radius ε in any plane normal to $\partial\Omega$, bounded by the tubular surface Σ_ε. The domain Ω is thus partitioned into $\Omega = \Omega_\varepsilon \cup (D_\varepsilon \setminus \Gamma)$, where $\Omega_\varepsilon = \Omega \setminus \bar{D}_\varepsilon$ and $\Gamma_\varepsilon = \Gamma \setminus \bar{D}_\varepsilon$. Upon introducing this splitting into Eq. (20), Eq. (26) is again obtained, with D and Σ replaced by D_ε and Σ_ε. Applying to that identity the divergence formula for the contribution of Ω_ε (i.e. away from the crack front, where this is legitimate) and invoking boundary conditions (2_3, 18_3), one obtains:

$$
\begin{aligned}
\frac{d\mathcal{J}}{db}(\Gamma) = &\int_0^T\!\!\int_{\Gamma_\varepsilon} \Big[\boldsymbol{\nabla}_S u_\Gamma . \boldsymbol{\nabla}_S v_\Gamma - \frac{1}{c^2}\dot{u}_\Gamma \dot{v}_\Gamma\Big]\theta_n \,\mathrm{d}S\,\mathrm{d}t \\
&+ \int_0^T\!\!\int_{\Sigma_\varepsilon} \Big[\Big(\boldsymbol{\nabla} u_\Gamma . \boldsymbol{\nabla} v_\Gamma - \frac{1}{c^2}\dot{u}_\Gamma \dot{v}_\Gamma\Big)\theta_n - (p_\Gamma \boldsymbol{\nabla} v_\Gamma + q_\Gamma \boldsymbol{\nabla} u_\Gamma).\boldsymbol{\theta}\Big] \,\mathrm{d}S\,\mathrm{d}t \\
&+ \int_0^T\!\!\int_{D_\varepsilon} \Big\{\Big[\boldsymbol{\nabla} u_\Gamma . \boldsymbol{\nabla} v_\Gamma - \frac{1}{c^2}\dot{u}_\Gamma \dot{v}_\Gamma\Big]\operatorname{div}\boldsymbol{\theta} - (\boldsymbol{\nabla} u_\Gamma \otimes \boldsymbol{\nabla} v_\Gamma + \boldsymbol{\nabla} v_\Gamma \otimes \boldsymbol{\nabla} u_\Gamma) : \boldsymbol{\nabla}\boldsymbol{\theta}\Big\} \,\mathrm{d}\Omega\,\mathrm{d}t \qquad (31)
\end{aligned}
$$

where $\boldsymbol{n}$ is the outward unit normal to Ω_ε.

Now, the limiting form when $\varepsilon \to 0$ of Eq. (31) is sought. In order to do so, one recalls that near the crack front the potential v admits the expansion:

$$
u = \sqrt{\frac{r}{2\pi}} K^u(s,t) \sin\frac{\phi}{2} + O(d) = u^s(r,\phi,z) + O(d) \qquad (32)
$$

and similarly for v with singularity factor $K^v(s,t)$; (r,ϕ) denote local polar coordinates, attached to a point $\boldsymbol{x}(s)$ of $\partial\Gamma$ characterized by its arc length s, in the plane orthogonal to $\partial\Gamma$ and emanating from $\boldsymbol{x}(s)$, and z is such that (r,ϕ,z) define cylindrical coordinates. Since by virtue of these expansions $\boldsymbol{\nabla} u . \boldsymbol{\nabla} v = O(1/r)$, the integral over D_ε vanishes in the limit ($\mathrm{d}V = r(1+O(r))\,\mathrm{d}r\mathrm{d}\phi\,\mathrm{d}s$ in D_ε). Moreover, it can be verified that $[\![\boldsymbol{\nabla} u . \boldsymbol{\nabla} v]\!] = O(r)$, and hence that the integral over Γ_ε becomes in the limit $\varepsilon \to 0$ the corresponding, convergent, integral over Γ. Finally, under mild smoothness assumptions on the closed curve $\partial\Gamma$ and the velocity field $\boldsymbol{\theta}$, one has:

$$
\begin{aligned}
&\int_0^T\!\!\int_{\Sigma_\varepsilon} \Big\{\Big[\boldsymbol{\nabla} u . \boldsymbol{\nabla} v - \frac{1}{c^2}\dot{u}\dot{v}\Big]\theta_n - (p\boldsymbol{\nabla} v + q\boldsymbol{\nabla} u).\boldsymbol{\theta}\Big\} \,\mathrm{d}S\,\mathrm{d}t \\
&\qquad = \int_0^T\!\!\int_{\partial\Gamma}\int_{-\pi}^{\pi} \Big\{[\boldsymbol{\nabla} u^s . \boldsymbol{\nabla} v^s]\theta_n(s) - (p^s \boldsymbol{\nabla} v^s + q^s \boldsymbol{\nabla} u^s).\boldsymbol{\theta}(s)\Big\}\varepsilon\mathrm{d}\phi\,\mathrm{d}s\,\mathrm{d}t + O(\varepsilon^{1/2})
\end{aligned}
$$

The integral in the right-hand side, which yields a finite contribution as the radius ε of the tubular neighbourhood goes to zero, can be evaluated in a straightforward way using expansions (32). This last calculation results in the following expression of $\mathrm{d}\mathcal{J}/\mathrm{d}b$:

$$
\frac{d\mathcal{J}}{db}(\Gamma) = -\frac{1}{4}\int_\Gamma \theta_n(s) \int_0^T K^u(s,t) K^v(s,t) \,\mathrm{d}t\,\mathrm{d}s \qquad (33)
$$

8 Extension to elastodynamics

The analysis conducted in the previous sections can be extended to linear elastodynamics in a straightforward way. The elastodynamic forward problem under consideration is such that the displacement $\boldsymbol{u}$, strain $\boldsymbol{\varepsilon}$ and stress $\boldsymbol{\sigma}$ are related by the field equations:

$$\operatorname{div}\boldsymbol{\sigma} - \rho\ddot{\boldsymbol{u}} = \mathbf{0} \qquad \boldsymbol{\sigma} = \boldsymbol{C}:\boldsymbol{\varepsilon} \qquad \boldsymbol{\varepsilon} = \frac{1}{2}(\boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}^T\boldsymbol{u}) \qquad \text{(in } \Omega) \tag{34}$$

($\boldsymbol{C}$: fourth-order elasticity tensor), the boundary conditions:

$$\boldsymbol{u} = \bar{\boldsymbol{u}} \quad \text{(on } S_u), \qquad \boldsymbol{p} = \bar{\boldsymbol{p}} \quad \text{(on } S_p), \qquad \boldsymbol{p} = \mathbf{0} \quad \text{(on } \Gamma), \tag{35}$$

(where $\boldsymbol{p} \equiv \boldsymbol{\sigma}.\boldsymbol{n}$ is the traction vector, defined in terms of the outward unit normal $\boldsymbol{n}$ to Ω) and the initial conditions:

$$\boldsymbol{u} = \dot{\boldsymbol{u}} = \mathbf{0} \qquad \text{(in } \Omega\text{, at } t = 0) \tag{36}$$

The generic objective function considered is of the form:

$$\mathcal{J}(\Gamma) = J(\boldsymbol{u}_\Gamma, \boldsymbol{p}_\Gamma, \Gamma) = \int_0^T\!\!\int_{S_p} \varphi_u(\boldsymbol{u}_\Gamma, \boldsymbol{x}, t)\,\mathrm{d}S\,\mathrm{d}t + \int_0^T\!\!\int_{S_u} \varphi_p(\boldsymbol{p}_\Gamma, \boldsymbol{x}, t)\,\mathrm{d}S\,\mathrm{d}t \tag{37}$$

8.1 Adjoint problem and domain integral formulation

The elastodynamic countarpart of the Lagrangian (13) is given by:

$$\begin{aligned}\mathcal{L}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{p}, \boldsymbol{q}, \Gamma) = J(\boldsymbol{u}, \boldsymbol{p}, \Gamma) &+ \int_0^T\!\!\int_\Omega [\boldsymbol{\sigma}:\boldsymbol{\nabla}\boldsymbol{v} + \rho\ddot{\boldsymbol{u}}.\boldsymbol{v}]\,\mathrm{d}V\,\mathrm{d}t \\ &- \int_0^T\!\!\int_{S_u} (\boldsymbol{u} - \bar{\boldsymbol{u}}).\tilde{\boldsymbol{p}}\,\mathrm{d}S\,\mathrm{d}t - \int_0^T\!\!\int_{S_u} \boldsymbol{p}.\boldsymbol{v}\,\mathrm{d}S\,\mathrm{d}t - \int_0^T\!\!\int_{S_p} \bar{\boldsymbol{p}}.\boldsymbol{v}\,\mathrm{d}S\,\mathrm{d}t\end{aligned} \tag{38}$$

where $(\boldsymbol{v}, \boldsymbol{q})$, the test functions of the forward problem in weak form, act as Lagrange multipliers. Then, the analysis of section 5 essentially repeats itself. The elastodynamic adjoint state $(\boldsymbol{v}, \boldsymbol{q})$ is found to solve the field equations (34), the boundary conditions:

$$\boldsymbol{q} = -\frac{\partial\varphi_u}{\partial\boldsymbol{u}} \quad \text{(on } S_p) \qquad \boldsymbol{v} = \frac{\partial\varphi_p}{\partial\boldsymbol{p}} \quad \text{(on } S_u) \qquad \boldsymbol{q} = \mathbf{0} \quad \text{(on } \Gamma^\pm) \tag{39}$$

and the final conditions:

$$\boldsymbol{v} = \dot{\boldsymbol{v}} = 0 \qquad \text{(in } \Omega\text{, at } t = T) \tag{40}$$

The derivative of J, expressed in domain integral form, is given by:

$$\begin{aligned}\frac{d\mathcal{J}}{db} &= \frac{d}{db}\mathcal{L}(\boldsymbol{u}_\Gamma, \boldsymbol{v}_\Gamma, \boldsymbol{p}_\Gamma, \boldsymbol{q}_\Gamma, \Gamma) \\ &= \int_0^T\!\!\int_\Omega \Big\{[\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma):\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \rho\ddot{\boldsymbol{u}}_\Gamma.\boldsymbol{v}_\Gamma]\operatorname{div}\boldsymbol{\theta} - [\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma).\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \boldsymbol{\sigma}(\boldsymbol{v}_\Gamma).\boldsymbol{\nabla}\boldsymbol{u}_\Gamma]:\boldsymbol{\nabla}\boldsymbol{\theta}\Big\}\,\mathrm{d}V\,\mathrm{d}t\end{aligned} \tag{41}$$

8.2 Shape sensitivity: boundary integral formulation (cavity problem)

The counterpart of identity (21), verified for any elastodynamic displacements $\boldsymbol{u}$ and $\boldsymbol{v}$ satisfying the field equation (34) and initial and final rest conditions, respectively, is:

$$\int_0^T \Big\{ [\boldsymbol{\sigma}(\boldsymbol{u}) : \boldsymbol{\nabla v} + \rho \ddot{\boldsymbol{u}}.\boldsymbol{v}] \text{div}\, \boldsymbol{\theta} - [\boldsymbol{\sigma}(\boldsymbol{u}).\boldsymbol{\nabla v} + \boldsymbol{\sigma}(\boldsymbol{v}).\boldsymbol{\nabla u}] : \boldsymbol{\nabla\theta} \Big\} \, \mathrm{d}t$$
$$= \int_0^T \text{div}\Big([\boldsymbol{\sigma}(\boldsymbol{u}) : \boldsymbol{\nabla v} - \rho \dot{\boldsymbol{u}}.\dot{\boldsymbol{v}}]\boldsymbol{\theta} - [\boldsymbol{\sigma}(\boldsymbol{u}).\boldsymbol{\nabla v} + \boldsymbol{\sigma}(\boldsymbol{v}).\boldsymbol{\nabla u}].\boldsymbol{\theta} \Big) \, \mathrm{d}t \quad (42)$$

This identity, when applied to (41) for the cavity problem, yields the following counterpart to (22):

$$\frac{d\mathcal{J}}{db} = \int_0^T \int_{\partial\Omega} \Big\{ [\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma) : \boldsymbol{\nabla v}_\Gamma - \rho \dot{\boldsymbol{u}}_\Gamma.\dot{\boldsymbol{v}}_\Gamma]\theta_n - [\boldsymbol{p}_\Gamma.\boldsymbol{\nabla v}_\Gamma + \boldsymbol{q}_\Gamma.\boldsymbol{\nabla u}_\Gamma].\boldsymbol{\theta} \Big\} \, \mathrm{d}S \, \mathrm{d}t \quad (43)$$

Since $\boldsymbol{\theta} = \boldsymbol{0}$ on S and $\boldsymbol{p} = \boldsymbol{q} = \boldsymbol{0}$ on Γ, the above equation reduces to:

$$\frac{d\mathcal{J}}{db} = \int_0^T \int_\Gamma [\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma) : \boldsymbol{\nabla v}_\Gamma - \rho \dot{\boldsymbol{u}}_\Gamma.\dot{\boldsymbol{v}}_\Gamma]\theta_n \, \mathrm{d}S \, \mathrm{d}t \quad (44)$$

The general expression of the bilinear form $\boldsymbol{\sigma}(\boldsymbol{u}) : \boldsymbol{\nabla v}$ in terms of $\boldsymbol{\nabla}_S \boldsymbol{u}$, $\boldsymbol{\nabla}_S \boldsymbol{v}$ and $\boldsymbol{p} = \boldsymbol{q}$ (assuming isotropic elasticity) is:

$$\boldsymbol{\sigma}(\boldsymbol{u}) : \boldsymbol{\nabla v} = \frac{1}{\mu} \Big\{ \boldsymbol{p}.\boldsymbol{q} - \frac{1}{2(1-\nu)} (\boldsymbol{p}.\boldsymbol{n}).(\boldsymbol{q}.\boldsymbol{n}) \Big\}$$
$$+ \mu \Big\{ \frac{2\nu}{1-\nu} \text{div}_S \boldsymbol{u} \, \text{div}_S \boldsymbol{v} + \frac{1}{2} (\boldsymbol{\nabla}_S \boldsymbol{u} + \boldsymbol{\nabla}_S^T \boldsymbol{u}) : (\boldsymbol{\nabla}_S \boldsymbol{v} + \boldsymbol{\nabla}_S^T \boldsymbol{v}) - (\boldsymbol{n}.\boldsymbol{\nabla}_S \boldsymbol{u}).(\boldsymbol{n}.\boldsymbol{\nabla}_S \boldsymbol{v}) \Big\} \quad (45)$$

where ν is the Poisson ratio and μ is the shear modulus. Since $\boldsymbol{p} = \boldsymbol{q} = \boldsymbol{0}$ on Γ, substitution of Eq. (45) into Eq. (43) produces an expression of $\mathrm{d}\mathcal{J}/\mathrm{d}b$ in terms of the fields $(\boldsymbol{u}, \boldsymbol{v})$ and their tangential derivatives, i.e. easily computable in a BEM framework.

8.3 Shape sensitivity: boundary integral formulation (crack problem)

Special cases of domain transformations. The treatment of Sec. 7.1 is then applicable to time-domain elastodynamics, using equation (41) together with the special form of $\boldsymbol{\theta}$ in D and equation (43) in $\Omega \setminus D$.

(a) Translation: the domain integral over D vanishes;

(b) Expansion: the domain integral over D becomes:

$$\eta \int_D \{ (m-2)\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma) : \boldsymbol{\nabla v}_\Gamma - m\rho \dot{\boldsymbol{u}}_\Gamma.\dot{\boldsymbol{v}}_\Gamma \} \, \mathrm{d}\Omega = \eta(m-2) \int_C \boldsymbol{p}_\Gamma.\boldsymbol{v}_\Gamma \, \mathrm{d}S - 2\rho\eta \int_D \dot{\boldsymbol{u}}_\Gamma.\dot{\boldsymbol{v}}_\Gamma \, \mathrm{d}\Omega$$

(c) Rotation: using the identity $\boldsymbol{\nabla w} = 2\boldsymbol{\varepsilon}(\boldsymbol{w}) - \boldsymbol{\nabla}^T \boldsymbol{w}$ (where $\boldsymbol{\varepsilon}(\boldsymbol{w})$: linearized strain tensor), the domain integral over D becomes, in component notation

$$\Omega_{aj} \int_D \{ \sigma_{ij}(\boldsymbol{u}) v_{a,j} + \sigma_{ij}(\boldsymbol{v}) u_{a,i} - 2[\sigma_{ij}(\boldsymbol{u})\varepsilon_{ai}(\boldsymbol{v}) + \sigma_{ij}(\boldsymbol{v})\varepsilon_{ai}(\boldsymbol{u})] \} \, \mathrm{d}\Omega \quad (46)$$

For isotropic elasticity (λ, μ: Lamé constants), one has

$$\sigma_{ij}(\boldsymbol{u})\varepsilon_{ai}(\boldsymbol{v}) + \sigma_{ij}(\boldsymbol{v})\varepsilon_{ai}(\boldsymbol{u}) = \lambda[(\operatorname{div}\boldsymbol{u})\varepsilon_{ja}(\boldsymbol{v}) + (\operatorname{div}\boldsymbol{v})\varepsilon_{ja}(\boldsymbol{u})] + 2\mu[\varepsilon_{ij}(\boldsymbol{u})\varepsilon_{ia}(\boldsymbol{v}) + \varepsilon_{ij}(\boldsymbol{v})\varepsilon_{ia}(\boldsymbol{u})]$$

which is symmetric with respect to the indices (a, j), so that the inner product of this quantity with Ω_{aj} vanishes. As a result, the integral over D, Eq. (46), becomes, after application of the divergence formula, integration in time over $[0, T]$ and using initial conditions on $\boldsymbol{u}$ and final conditions on $\boldsymbol{v}$:

$$\Omega_{aj}\int_0^T\int_C [p_i(\boldsymbol{u})v_a + p_i(\boldsymbol{v})u_a]\,\mathrm{d}S\,\mathrm{d}t + \Omega_{aj}\int_0^T\int_D [\dot{u}_a\dot{v}_j + \dot{u}_j\dot{v}_a]\,\mathrm{d}\Omega\,\mathrm{d}t$$

But the second integral in the above equation is symmetric with respect to the indices (a, j); thus its inner product with Ω_{aj} vanishes and only the first term remains.

Collecting all results, we have respectively for cases (a), (b) and (c):

$$\frac{d\mathcal{J}}{db} = \begin{cases} I(\boldsymbol{u}_\Gamma, \boldsymbol{v}_\Gamma, \boldsymbol{\theta}_0, C) & \text{(translation)} \\ I(\boldsymbol{u}_\Gamma, \boldsymbol{v}_\Gamma, \eta\boldsymbol{x}, C) + \eta(m-2)\displaystyle\int_0^T\int_C \boldsymbol{p}_\Gamma.\boldsymbol{v}_\Gamma\,\mathrm{d}S\,\mathrm{d}t - 2\rho\eta\int_0^T\int_D \dot{\boldsymbol{u}}_\Gamma.\dot{\boldsymbol{v}}_\Gamma\,\mathrm{d}\Omega\,\mathrm{d}t & \text{(expansion)} \\ I(\boldsymbol{u}_\Gamma, \boldsymbol{v}_\Gamma, \boldsymbol{\omega}.\boldsymbol{x}, C) + \displaystyle\int_0^T\int_C [\boldsymbol{p}_\Gamma\otimes\boldsymbol{v}_\Gamma + \boldsymbol{q}_\Gamma\otimes\boldsymbol{u}_\Gamma].\boldsymbol{\omega}\,\mathrm{d}S\,\mathrm{d}t & \text{(rotation)} \end{cases}$$

where

$$I(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{\theta}, C) = \int_0^T\int_C \Big\{[\rho\dot{\boldsymbol{u}}_\Gamma.\dot{\boldsymbol{v}}_\Gamma - \boldsymbol{\sigma}(\boldsymbol{u}_\Gamma):\boldsymbol{\nabla}\boldsymbol{v}_\Gamma]\theta_n + [\boldsymbol{p}_\Gamma.\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \boldsymbol{q}_\Gamma.\boldsymbol{\nabla}\boldsymbol{u}_\Gamma].\boldsymbol{\theta}\Big\}\,\mathrm{d}S\,\mathrm{d}t$$

Additive decomposition of transformation velocity near the crack front. In the same way as in section 7.2, and using the same notations, Eq. (41) can be split according to:

$$\begin{aligned}\frac{d\mathcal{J}}{db} &= \int_0^T\int_{\tilde{\Omega}} \Big\{[\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma):\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \rho\ddot{\boldsymbol{u}}_\Gamma).\boldsymbol{v}_\Gamma]\operatorname{div}\boldsymbol{\theta} - [\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma).\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \boldsymbol{\sigma}(\boldsymbol{v}_\Gamma.\boldsymbol{\nabla}\boldsymbol{u}_\Gamma]:\boldsymbol{\nabla}\boldsymbol{\theta}\Big\}\,\mathrm{d}V\,\mathrm{d}t \\ &+ \int_0^T\int_D \Big\{[\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma):\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \rho\ddot{\boldsymbol{u}}_\Gamma.\boldsymbol{v}_\Gamma]\operatorname{div}\boldsymbol{\theta} - [\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma).\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \boldsymbol{\sigma}(\boldsymbol{v}_\Gamma).\boldsymbol{\nabla}\boldsymbol{u}_\Gamma]:\boldsymbol{\nabla}\boldsymbol{\mu}\Big\}\,\mathrm{d}V\,\mathrm{d}t \\ &+ \int_0^T\int_D \Big\{[\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma):\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \rho\ddot{\boldsymbol{u}}_\Gamma.\boldsymbol{v}_\Gamma]\operatorname{div}\tilde{\boldsymbol{\theta}} - [\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma).\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \boldsymbol{\sigma}(\boldsymbol{v}_\Gamma).\boldsymbol{\nabla}\boldsymbol{u}_\Gamma]:\boldsymbol{\nabla}\tilde{\boldsymbol{\theta}}\Big\}\,\mathrm{d}V\,\mathrm{d}t \end{aligned} \tag{47}$$

and identity (42) followed by an application of the divergence formula to the first two integrals yields the elastodynamic counterpart of Eq. (28):

$$\begin{aligned}\frac{d\mathcal{J}}{db} &= \int_0^T\int_\Gamma \Big\{[\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma):\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \rho\ddot{\boldsymbol{u}}_\Gamma.\boldsymbol{v}_\Gamma](\boldsymbol{\mu}.\boldsymbol{n}) - [\boldsymbol{p}_\Gamma.\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \boldsymbol{q}_\Gamma.\boldsymbol{\nabla}\boldsymbol{u}_\Gamma].\boldsymbol{\mu}\Big\}\,\mathrm{d}S\,\mathrm{d}t \\ &+ \int_0^T\int_\Sigma \Big\{[\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma):\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \rho\ddot{\boldsymbol{u}}_\Gamma.\boldsymbol{v}_\Gamma](\tilde{\boldsymbol{\theta}}.\boldsymbol{n}) - [\boldsymbol{p}_\Gamma.\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \boldsymbol{q}_\Gamma.\boldsymbol{\nabla}\boldsymbol{u}_\Gamma].\tilde{\boldsymbol{\theta}}\Big\}\,\mathrm{d}S\,\mathrm{d}t \\ &+ \int_0^T\int_D \Big\{[\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma):\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \rho\ddot{\boldsymbol{u}}_\Gamma.\boldsymbol{v}_\Gamma]\operatorname{div}\tilde{\boldsymbol{\theta}} - [\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma).\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \tilde{\boldsymbol{\sigma}}(\boldsymbol{v}_\Gamma).\boldsymbol{\nabla}\boldsymbol{u}_\Gamma]:\boldsymbol{\nabla}\tilde{\boldsymbol{\theta}}\Big\}\,\mathrm{d}V\,\mathrm{d}t \end{aligned} \tag{48}$$

Sensitivity formulation in terms of stress intensity factors. Using the same notations as in section 7.3, the limiting case for $\varepsilon \to 0$ of

$$\begin{aligned}\frac{d\mathcal{J}}{db} &= \int_0^T\!\!\int_{\Sigma_\varepsilon} \Big\{[\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma)\!:\!\boldsymbol{\nabla}\boldsymbol{v}_\Gamma - \rho\dot{\boldsymbol{u}}_\Gamma.\dot{\boldsymbol{v}}_\Gamma]\theta_n - [\boldsymbol{p}_\Gamma.\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \boldsymbol{q}_\Gamma.\boldsymbol{\nabla}\boldsymbol{u}_\Gamma].\boldsymbol{\theta}\Big\}\,\mathrm{d}S\,\mathrm{d}t \\ &+ \int_0^T\!\!\int_{\Gamma_\varepsilon} [\![\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma)\!:\!\boldsymbol{\nabla}\boldsymbol{v}_\Gamma - \rho\dot{\boldsymbol{u}}_\Gamma.\dot{\boldsymbol{v}}_\Gamma]\!]\theta_n\,\mathrm{d}S\,\mathrm{d}t \\ &+ \int_0^T\!\!\int_{D_\varepsilon} \Big\{[\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma)\!:\!\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \rho\ddot{\boldsymbol{u}}_\Gamma.\boldsymbol{v}_\Gamma]\mathrm{div}\,\boldsymbol{\theta} - [\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma).\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \boldsymbol{\sigma}(\boldsymbol{v}_\Gamma).\boldsymbol{\nabla}\boldsymbol{u}_\Gamma]\!:\!\boldsymbol{\nabla}\boldsymbol{\theta}\Big\}\,\mathrm{d}V\,\mathrm{d}t \qquad (49)\end{aligned}$$

is sought. In order to do so, the well-known expansions of the forward displacement field near the crack front (assuming isotropic elasticity) is used:

$$\begin{aligned} u_r &= \frac{1}{2\mu}\sqrt{\frac{r}{2\pi}}\Big[K_I^u(s,t)\cos\frac{\phi}{2}(3-4\nu-\cos\phi) + K_{II}^u(s,t)\sin\frac{\phi}{2}(4\nu-1+3\cos\phi)\Big] + O(r) \\ &= u_r^S(r,\phi,s) + O(r) \\ u_\phi &= \frac{1}{2\mu}\sqrt{\frac{r}{2\pi}}\Big[-K_I^u(s,t)\sin\frac{\phi}{2}(1-4\nu-3\cos\phi) + K_{II}^u(s,t)\cos\frac{\phi}{2}(4\nu-5+3\cos\phi)\Big] + O(r) \qquad (50) \\ &= u_\phi^S(r,\phi,s) + O(r) \\ u_z &= \frac{2K_{III}^u(s,t)}{\mu}\sqrt{\frac{r}{2\pi}}\sin\frac{\phi}{2} + O(r) = u_z^S(r,\phi,s) + O(r)\end{aligned}$$

and similarly for $\boldsymbol{v}$ with stress intensity factors $K^v_{I,II,III}$ and leading term $\boldsymbol{v}^S$. Since by virtue of these expansions $\boldsymbol{\sigma}(\boldsymbol{u})\!:\!\boldsymbol{\nabla}\boldsymbol{v}$ and $\boldsymbol{\sigma}(\boldsymbol{v})\!:\!\boldsymbol{\nabla}\boldsymbol{u}$ are $O(1/r)$, the integral over D_ε vanishes in the limit ($\mathrm{d}V = r(1+O(r))\,\mathrm{d}r\mathrm{d}\phi\,\mathrm{d}s$ in D_ε). Besides, it can be verified that $[\![\boldsymbol{\sigma}^S\!:\!\boldsymbol{\nabla}\boldsymbol{v}^S]\!] = O(d)$, and hence that the integral over Γ_ε becomes in the limit $\varepsilon \to 0$ the corresponding, convergent, integral over Γ. Finally, under mild smoothness assumptions on the closed curve $\partial\Gamma$ and the velocity field $\boldsymbol{\theta}$, one has:

$$\begin{aligned}&\int_0^T\!\!\int_{\Sigma_\varepsilon} \Big\{[\boldsymbol{\sigma}(\boldsymbol{u}_\Gamma)\!:\!\boldsymbol{\nabla}\boldsymbol{v}_\Gamma - \rho\dot{\boldsymbol{u}}_\Gamma.\dot{\boldsymbol{v}}_\Gamma]\theta_n - [\boldsymbol{p}_\Gamma.\boldsymbol{\nabla}\boldsymbol{v}_\Gamma + \boldsymbol{q}_\Gamma.\boldsymbol{\nabla}\boldsymbol{u}_\Gamma].\boldsymbol{\theta}\Big\}\,\mathrm{d}S\,\mathrm{d}t \\ &\qquad = \int_0^T\!\!\int_{\partial\Gamma}\int_{-\pi}^{\pi} \Big\{[\boldsymbol{\sigma}^S\!:\!\boldsymbol{\nabla}\boldsymbol{v}^S]\theta_n(s) - [\boldsymbol{p}^S.\boldsymbol{\nabla}\boldsymbol{v}^S + \boldsymbol{q}^S.\boldsymbol{\nabla}\boldsymbol{u}^S].\boldsymbol{\theta}(s)\Big\}\varepsilon\mathrm{d}\phi\,\mathrm{d}s\,\mathrm{d}t + O(\varepsilon^{1/2})\end{aligned}$$

The integral in the right-hand side, which yields a finite contribution as the radius ε of the tubular neighbourhood goes to zero, can be evaluated in a straightforward way using expansions (50). This last calculation results in the following expression of $\mathrm{d}\mathcal{J}/\mathrm{d}b$, counterpart of Eq. (33):

$$\begin{aligned}\frac{d\mathcal{J}}{db} &= \int_\Gamma \theta_n(s)\int_0^T [\![\boldsymbol{\sigma}\!:\!\boldsymbol{\nabla}\boldsymbol{v} - \rho\dot{\boldsymbol{u}}.\dot{\boldsymbol{v}}]\!]\,\mathrm{d}t\,\mathrm{d}S \\ &- \frac{1}{\mu}\int_{\partial\Gamma}\theta_\nu(s)\int_0^T \Big\{(1-\nu)[K_I^uK_I^v + K_{II}^uK_{II}^v] + K_{III}^uK_{III}^v\Big\}(s,t)\,\mathrm{d}t\,\mathrm{d}s \\ &+ \frac{1-\nu}{\mu}\int_{\partial\Gamma}\theta_n(s)\int_0^T (K_I^uK_{II}^v + K_{II}^uK_I^v)(s,t)\,\mathrm{d}t\,\mathrm{d}s \qquad (51)\end{aligned}$$

having put $\theta_\nu = \boldsymbol{\theta}.\boldsymbol{\nu}$, where $\boldsymbol{\nu}(s)$ denotes the unit outward normal to $\partial\Gamma$ lying in the tangent plane to Γ at $\boldsymbol{x}(s)$.

9 Numerical examples

To illustrate concepts developed in this paper, the computation of sensitivities with respect to shape perturbations of either a hole (example 1, Fig. 6a) or a crack (example 2, Fig. 7a) in an elastic plate are presented. In both cases, the plate has linearly elastic and isotropic constitutive properties (Young modulus $E = 200$ GPa, Poisson ratio $\nu = 0.3$, mass density $\rho = 5000$ kg/m^3), plane strain conditions and dynamical loading are assumed. The forward problem is solved by a 2D time-domain dual-reciprocity elastodynamic BEM.

The objective function J is defined for both examples as:

$$\mathcal{J}(\Gamma) = -\frac{1}{2}\int_0^T\int_{S_m} u_1^2(\boldsymbol{x},t)\,\mathrm{d}S\,\mathrm{d}t \tag{52}$$

where $u_1(\boldsymbol{x},t)$ indicates displacements in x_1 direction of nodes on the boundary $S_m = \mathrm{MN}\cup\mathrm{OP}$ at time t (Figs. 6 and 7). Sensitivities for example 1 and 2 are computed using equation (43) and (51), respectively, and compared with the first-order derivative of the second-degree polynomial approximation of J with respect to the relevant shape parameter b.

9.1 Example 1

The first-order derivative of the objective function (52) with respect to a transformation parameter p of the cavity is calculated for the rectangular plate shown in Fig. 6a. Two kinds of transformations of the cavity are condsidered: translation along the x_1 direction

$$\boldsymbol{\Phi}(\boldsymbol{x},b) = \boldsymbol{x} + b\boldsymbol{e}_1 \tag{53}$$

(where $\boldsymbol{e}_1$ is a unit vector along the x_1-direction) and expansion

$$\boldsymbol{\Phi}(\boldsymbol{x},b) = (1+b)\boldsymbol{x} \tag{54}$$

(in both cases, $\boldsymbol{x}$ denotes a point on the cavity boundary). The external boundary of the plate was discretized using 32 (for case I) or 48 (for cases II and III) continous quadratic boundary elements of uniform length, where cases I to III refer to Table 1. In all three cases, 10 continous quadratic boundary elements of uniform length were used for the cavity boundary, as well as 104 domain points. The number of sensor points was 32 (case I) or 64 (cases II and III). The distribution of the boundary nodes and the domain points is depicted for case I in Fig 6b.

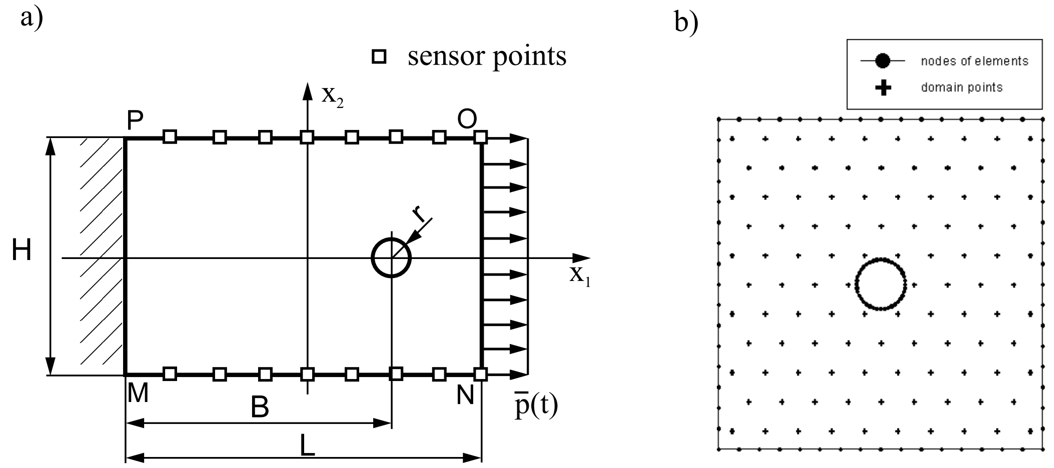

Figure 6: Example 1 (plate with a cavity): (a) geometrical configuration and notation; (b) boundary element model (case I in Table 1).

The results are presented, together with the corresponding derivatives calculated from a polynomial approximation of J, in Table 1 for three cases of plate geometry and loading (using the geometrical notations of Fig. 6a).

9.2 Example 2

The first-order derivative of the objective function (52) with respect to a transformation parameter p of the crack is calculated for the rectangular plate shown in Fig. 7a, which contains an initially straight crack. Two kinds of transformations of the crack are condsidered: translation along the

Case	Geometry and load	Transformation	Sensitivity analysis		
			$\mathrm{d}\mathcal{J}/\mathrm{d}b$	$\Delta J/\Delta b$	error
I	$L\!=\!H\!=\!20,\ B\!=\!10,\ r\!=\!1$ (mm)				
	$\bar{p}(t) = \bar{p}_0 H(t)$ $(\bar{p}_0 = 0.4\,\mathrm{MN/mm})$	translation x_1	0.0280	0.0275	1.8%
	$0 \leq t \leq T = 80\mu s$ $(\Delta t = 0.2\mu s)$	expansion	-1.161	-1.223	0.5%
II	$L\!=\!40,\ H\!=\!20,\ B\!=\!30,\ r\!=\!1$ (mm)				
	$\bar{p}(t) = \bar{p}_0 H(t)$ $(\bar{p}_0 = 0.4\,\mathrm{MN/mm})$	translation x_1	0.932	0.911	2.3%
	$0 \leq t \leq T = 80\mu s$ $(\Delta t = 0.2\mu s)$	expansion	-1.916	-1.949	1.7%
III	$L\!=\!40,\ H\!=\!20,\ B\!=\!30,\ r\!=\!1$ (mm)				
	$\bar{p}(t) = \bar{p}_0 sin\omega t + \bar{p}_0$	translation x_1	2.6005E-6	2.6029E-6	1.0%
	$(\bar{p}_0 = 50\,\mathrm{N/mm},\ \omega = 79kHz)$				
	$0 \leq t \leq T = 80\mu s$ $(\Delta t = 0.2\mu s)$	expansion	-3.69E-6	-3.65E-6	0.9%

Table 1: Example 1: Sensitivity results for various cavity perturbations.

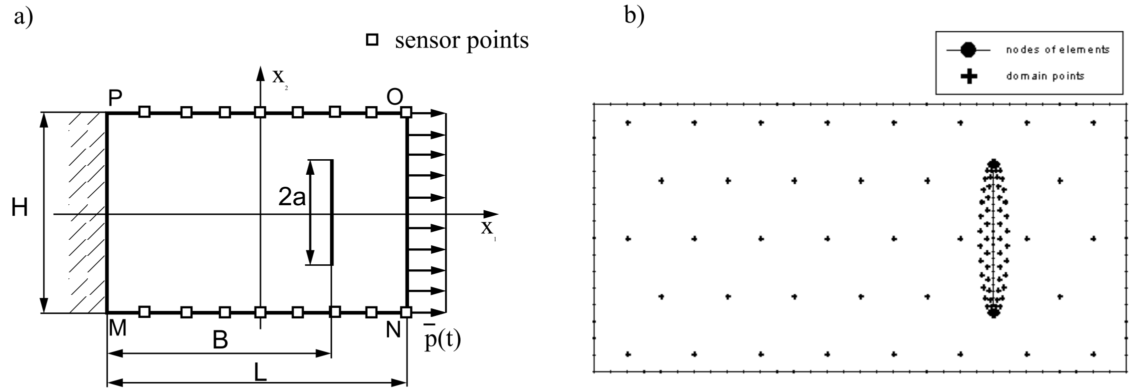

Figure 7: Example 2 (plate with a crack): (a) geometrical configuration and notation; (b) boundary element model (case II in Table 1).

x_1 direction (again according to Eq. (53)) and a deformation into parabolic shape according to:

$$\mathbf{\Phi}(\boldsymbol{x}, p) = \boldsymbol{x} + b(a^2 - x_2^2) \tag{55}$$

where a is the initial half-length of the crack. The external boundary of the plate was discretized using 32 (for case I) or 48 (for cases II and III) continous quadratic boundary elements of uniform length, where cases I to III refer to Table 2. In all three cases, 20 discontinuous quadratic boundary elements were used for the crack (with their lengths graded so that elements closer to the crack tips are shorter), as well as 100 domain points. The number of sensor points was 32 (case I) or 64 (cases II and III). The distribution of the boundary nodes and the domain points is depicted for case II in Fig 7b).

The results of derivatives are presented in Table 2 for three cases of geometry and loading of the plate, together with the corresponding derivatives calculated from a polynomial approximation

Case	Geometry and load	Transformation	Sensitivity analysis		
			$\mathrm{d}\mathcal{J}/\mathrm{d}b$	$\Delta J/\Delta b$	error
I	$L\!=\!H\!=\!20$, $B\!=\!10$, $a\!=\!2.5$ (mm)				
	$\bar{p}(t) = \bar{p}_0 H(t)$ ($\bar{p}_0 = 0.4\,\mathrm{MN/mm}$)	translation x_1	10.359	10.445	0.8%
	$0 \le t \le T = 80\mu s$ ($\Delta t = 0.2\mu s$)	parabolic	0.493	0.479	2.9%
II	$L\!=\!40$, $H\!=\!20$, $B\!=\!30$, $a\!=\!2.5$ (mm)				
	$\bar{p}(t) = \bar{p}_0 H(t)$ ($\bar{p}_0 = 0.4\,\mathrm{MN/mm}$)	translation x_1	24.730	24.531	0.8%
	$0 \le t \le T = 80\mu s$ ($\Delta t = 0.2\mu s$)	parabolic	1.355	1.332	1.7%
III	$L\!=\!40$, $H\!=\!20$, $B\!=\!30$, $a\!=\!2.5$ (mm)				
	$\bar{p}(t) = \bar{p}_0 sin\omega t + \bar{p}_0$	translation x_1	2.474E-4	2.497E-4	1.0%
	($\bar{p}_0 = 200\,\mathrm{N/mm}$, $\omega = 1257kHz$)				
	$0 \le t \le T = 20\mu s$ ($\Delta t = 0.2\mu s$)	parabolic	2.050E-5	2.053E-5	0.3%

Table 2: Example 2: sensitivity results for various crack perturbations.

of J (using the geometrical notations of Fig. 7a).

10 Discussion and concluding remarks

In the present work a shape sensitivity analysis for identification of internal cavities or cracks has been presented. The main motivation of this paper was to explore the adjoint variable approach, in the presence of cracks and in connexion with BIE formulations of the forward problem.

First, a general formulation for the sensitivity with respect to the shape of a cavity of objective functionals expressed as boundary integrals has been derived using the material derivative-adjoint variable approach. The sensitivity of the functional has been expressed as a boundary integral.

In the case of a crack, the previous boundary-only expression is not applicable. However, revisiting the discussion of the cavity problem, it has been shown that for two classes of crack perturbations the adjoint variable approach to sensitivity analysis is still applicable in the presence of cracks. Firstly, when the domain transformations considered consist of translation, rotation or expansion of the crack, the functional sensitivity is expressed as an integral over an arbitrary surface surrounding the crack, supplemented for the case of crack expansion in dynamics by a domain integral over the crack front neighbourhood enclosed by this surface. This applies for arbitrary geometries, either three- and two-dimensional. Earlier works on path-independent integral approach to sensitivity analysis are thus revisited and generalized. Secondly, sensitivity formulas applicable to arbitrary shape perturbations were established by means of an additive decomposition of the transformation velocity over a tubular neighbourhood of the crack front. Thirdly, the limiting case of the latter results when the tubular neighbourhood shrinks around the crack front has been shown to yield a boundary-only sensitivity formula involving the stress intensity factors of both the forward and the adjoint solutions. All these results were obtained in connection with both scalar wave and elastodynamic problems formulated in the time domain.

The analysis conducted in this paper is applicable without difficulty to objective functions of the form:

$$\mathcal{J}(\Gamma) = J(u_\Gamma, p_\Gamma, \Gamma) = \int_0^T \int_{S_p} \varphi_u(u_\Gamma, \boldsymbol{x}, t) \, \mathrm{d}S \, \mathrm{d}t + \int_0^T \int_{S_u} \varphi_p(p_\Gamma, \boldsymbol{x}, t) \, \mathrm{d}S \, \mathrm{d}t + \int_\Gamma \psi(\boldsymbol{x}) \, \mathrm{d}S \qquad (56)$$

where the last integral might for instance be used to formulate some *a priori* information about the defect (for instance by penalizing high curvatures to avoid recovering oscillatory shapes). Since this last integral depends on Γ in an explicit manner, one simply needs to invoke the differentiation formula (12). As a result, the contribution

$$\int_\Gamma [\boldsymbol{\nabla}\psi.\boldsymbol{\theta} + \psi \mathrm{div}_S \boldsymbol{\theta}] \, \mathrm{d}S$$

should be added to each of the sensitivity formulas (20), (22), (23), (24), (25), (26), (28), (29), (30), (31), (33), (41), (43), (44), (47), (48), 49), (51).

It is important to stress that Eq. (51) provides the sensitivity of an integral functional to a *perturbation of a fixed crack configuration*, not a crack propagation, hence the use of expansions (50), valid for a crack which does not physically propagate.

Equation (51) is also applicable, with straightforward modifications, to elastostatics and elastodynamics in the frequency domain. For instance, in elastostatics, $\mathcal{J}(\Gamma)$ is the potential energy at equilibrium for the particular choice $\varphi_u = -(\bar{\boldsymbol{p}}.\boldsymbol{u})/2$, $\varphi_p = (\bar{\boldsymbol{u}}.\boldsymbol{p})/2$ in Eq. (5). For this special case, the adjoint solution turns out to be $\tilde{\boldsymbol{u}} = (1/2)\boldsymbol{u}$, i.e. $K_I^v = K_I^u/2$, etc. In equation (51), the factor of $\theta_\nu(s)$ turns out to be, as expected, minus the energy release rate $G(s)$, i.e. minus the J_1-integral, whereas the factor of $\theta_n(s)$ is the 3-D generalization of the J_2-integral (Budiansky and Rice, 1973; Bui, 1978). Finally, with the choice $S_p = S, s_u = \emptyset$ and $\varphi_p = \bar{\boldsymbol{p}}.\hat{\boldsymbol{u}} - \boldsymbol{u}.\hat{\boldsymbol{p}}$, where $\hat{\boldsymbol{u}}, \hat{\boldsymbol{p}}$ are the boundary traces of a *pre-selected* auxiliary elastodynamic state with *final* homogeneous conditions, one finds that $\tilde{\boldsymbol{u}} = \hat{\boldsymbol{u}}$ and that the factor of $\theta_\nu(s)$ in (51) is the 3-D generalization of the so-called H-integral (Bui and Maigre, 1988).

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